2-hydroxy-3-methyl-2-(propan-2-yl)butanoic acid
5438-17-5 | DTXSID50280375

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 59.5 °C

Global applicability domain: Inside

Local applicability domain index: 4.90e-01

Confidence level: 5.74e-01

Nearest Neighbors from the Training Set

Image not found
(9Z,12R)-12-Hydroxyoctadec-9-enoic acid
Measured: 5.50
Predicted: 24.7

Image not found
16-Hydroxypalmitic acid
Measured: 98.0
Predicted: 82.5

Image not found
11-Hydroxyundecanoic acid
Measured: 65.5
Predicted: 71.0